Ethyl orthoformate 122-51-0 | DTXSID8041957

Model	Perforn	nance
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Model	Data	
Model	Dala	

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.72	51.8	0.74	50.3	0.73	52.7	

Model Results

Predicted value: -38.9 °C

Global applicability domain: Inside

Local applicability domain index: 8.21e-01

Confidence level: 4.33e-01

Nearest Neighbors from the Training Set

Image not found

Diethylene glycol diethyl ether

Measured: -45.0 Predicted: -34.4

Image not found

Bis(2-methoxyethyl) ether

Measured: -68.0 Predicted: -51.9

Image not found

1,1,3-Triethoxypropane

Measured: 53.0 Predicted: -13.4

Image not found

Diethylene glycol dibutyl ether

Measured: -60.0 Predicted: -51.7